checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1_cr1_pristine_a

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 1_cr1_pristine_a

Bond precision: N- C = 0.0066 A Wavelength=0.68890

Cell: a=8.9201(5) b=9.3166(6) c=9.7444(7)
alpha=86.900(6) beta=81.977(6) gamma=70.807(6)
Temperature: 30 K

	Calculated	Reported
Volume	757.28(9)	757.28(9)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C7 Mo N7, 0.179(O2), 1.641(O), 4(K)	C7 K4 Mo N7 O2
Sum formula	C7 K4 Mo N7 O2	C7 K4 Mo N7 O2
Mr	466.48	466.48
Dx,g cm-3	2.046	2.046
Z	2	2
Mu (mm-1)	1.795	1.795
F000	450.0	450.0
F000'	447.80	
h,k,lmax	12,13,13	12,13,13
Nref	4421	4004
Tmin,Tmax	0.937,0.982	0.998,1.000
Tmin'	0.914	

Correction method= # Reported T Limits: Tmin=0.998 Tmax=1.000
AbsCorr = EMPIRICAL

Data completeness= 0.906 Theta(max)= 28.987

R(reflections)= 0.0506(2753) wR2(reflections)= 0.1292(4004)

S = 1.022 Npar= 200

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level A

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 0.79Ang From Mo1A 3.57 eA-3

Author Response: The residual density near molybdenum is due to partial photoinduced changes in the crystal structure caused by a strong synchrotron X-ray source.

Alert level B

PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O1A Check

Author Response: The water molecules in the structure are disordered, so we decided not to model the positions of the hydrogen atoms, since the refinement led to an unphysical result.

Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low . 0.979 Why?
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
Calc: C7 Mo N7, 0.179(O2), 1.641(O), 4(K)
Rep.: C7 K4 Mo N7 O2
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 3.13 Report
PLAT097_ALERT_2_C Large Reported Max. (Positive) Residual Density 3.82 eA-3
PLAT213_ALERT_2_C Atom N7A has ADP max/min Ratio ..... 3.1 prolat
PLAT220_ALERT_2_C NonSolvent Resd 1 N Ueq(max)/Ueq(min) Range 3.9 Ratio
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 58 Report

1	8	3,	-6	1	4,	2	8	4,	3	8	4,	4	8	4,	-5	0	6,
-5	1	6,	-4	1	7,	-4	2	7,	1	7	7,	-3	1	8,	-1	4	8,
0	4	8,	-1	5	8,	0	5	8,	1	5	8,	-1	6	8,	0	6	8,
1	6	8,	-1	7	8,	0	7	8,	2	-1	9,	3	0	9,	3	1	9,
3	2	9,	-2	3	9,	-1	3	9,	3	3	9,	-2	4	9,	-1	4	9,
0	4	9,	1	4	9,	-2	5	9,	-1	5	9,	0	5	9,	1	5	9,
2	5	9,	-1	6	9,	0	6	9,	1	6	9,	2	6	9,	1	7	9,
2	7	9,	-2	3	10,	-1	3	10,	0	3	10,	1	3	10,	-1	4	10,
0	4	10,	1	4	10,	0	5	10,	1	5	10,	2	5	10,	2	6	10,
3	6	10,	0	3	11,	1	3	11,	2	4	11,						

PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.83Ang From O1A . 0.63 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.97Ang From O1A . 0.59 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.89Ang From N1A . 0.59 eA-3

Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu

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               not performed for this radiation type.
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound ..     Please Check
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)      0.006 Degree
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    2)       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    4)       100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    2)       0.72 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    4)       0.64 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....        O2A Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          3 Note
               O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          4 Note
               O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          5 Note
               K
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          6 Note
               K
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters         1 Info
PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary ..     Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).         1 Note
                 0  0  1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        358 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity .....              3.6 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value .....           1.441 Note
               Predicted wR2: Based on SigI**2  8.96 or SHELX Weight 12.65
PLAT984_ALERT_1_G The  K-f'=    0.1938 Deviates from the B&C-Value     0.1927 Check
PLAT984_ALERT_1_G The Mo-f'=   -1.8748 Deviates from the B&C-Value    -1.8622 Check
PLAT985_ALERT_1_G The  K-f"=    0.2386 Deviates from the B&C-Value     0.2361 Check
PLAT985_ALERT_1_G The Mo-f"=    0.6623 Deviates from the B&C-Value     0.6534 Check
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1 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
11 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
22 **ALERT level G** = General information/check it is not something unexpected

10 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
10 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
10 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 19/12/2024; check.def file version of 19/12/2024

Datablock 1_cr1_pristine_a - ellipsoid plot